

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
 Data File : VN075840.D
 Acq On : 16 Dec 2022 12:13
 Operator : JC\MD
 Sample : N6036-01
 Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31916

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075840.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.171	1030	1040	1044	rBV	203655	479380	26.39%	1.553%
2	8.224	1044	1049	1066	rVB	412883	911264	50.17%	2.951%
3	8.582	1099	1110	1122	rBV	206742	465986	25.66%	1.509%
4	9.100	1188	1198	1210	rBV	526535	1091091	60.07%	3.534%
5	10.571	1439	1448	1455	rBV	782654	1454838	80.10%	4.712%
6	10.635	1455	1459	1466	rVB	16406	32312	1.78%	0.105%
7	11.871	1660	1669	1679	rBV	677573	1207068	66.46%	3.909%
8	12.076	1696	1704	1709	rBV3	37481	65364	3.60%	0.212%
9	12.400	1749	1759	1766	rBV4	17355	52953	2.92%	0.172%
10	12.488	1766	1774	1778	rVB2	21034	34501	1.90%	0.112%
11	12.606	1781	1794	1803	rBV7	15842	60579	3.34%	0.196%
12	12.706	1806	1811	1814	rBV5	13938	29151	1.60%	0.094%
13	12.770	1819	1822	1825	rVV2	24468	41190	2.27%	0.133%
14	12.800	1825	1827	1830	rVV3	24271	29563	1.63%	0.096%
15	12.853	1830	1836	1845	rVB	537847	917584	50.52%	2.972%
16	13.035	1861	1867	1872	rVB	27113	51233	2.82%	0.166%
17	13.100	1872	1878	1881	rBV	70179	122799	6.76%	0.398%
18	13.165	1881	1889	1896	rVV2	230056	487769	26.86%	1.580%
19	13.229	1896	1900	1903	rVB3	19527	29222	1.61%	0.095%
20	13.341	1910	1919	1925	rBV2	51508	163746	9.02%	0.530%
21	13.400	1925	1929	1934	rVB2	77398	118223	6.51%	0.383%
22	13.488	1936	1944	1948	rBV	140822	242621	13.36%	0.786%
23	13.541	1948	1953	1957	rVB	84694	129939	7.15%	0.421%
24	13.617	1963	1966	1970	rVB3	36006	48506	2.67%	0.157%
25	13.676	1971	1976	1981	rBV3	100802	192994	10.63%	0.625%
26	13.723	1981	1984	1991	rVV4	77485	153107	8.43%	0.496%
27	13.794	1991	1996	2004	rVB2	718864	1291026	71.08%	4.181%
28	13.870	2004	2009	2015	rVB3	101604	219267	12.07%	0.710%
29	13.959	2018	2024	2025	rBV5	57059	95664	5.27%	0.310%
30	13.988	2025	2029	2032	rVV2	187990	277638	15.29%	0.899%
31	14.023	2032	2035	2045	rVB3	200473	468808	25.81%	1.518%
32	14.106	2045	2049	2055	rBV	498328	815471	44.90%	2.641%
33	14.188	2055	2063	2067	rVV2	109727	177798	9.79%	0.576%
34	14.253	2069	2074	2075	rVV	143054	190971	10.51%	0.619%
35	14.276	2076	2078	2082	rVB	185038	218388	12.02%	0.707%
36	14.335	2083	2088	2092	rBV	237303	366119	20.16%	1.186%

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37	14.447	2100	2107	2111	rBV2	284640	514815	28.34%	1.667%
38	14.523	2112	2120	2124	rVB5	76122	160562	8.84%	0.520%
39	14.582	2125	2130	2134	rBV3	165182	319055	17.57%	1.033%
40	14.629	2134	2138	2141	rVV4	249407	368739	20.30%	1.194%
41	14.664	2141	2144	2147	rVV2	163419	229304	12.62%	0.743%
42	14.700	2147	2150	2153	rVB	198767	231959	12.77%	0.751%
43	14.735	2153	2156	2160	rVB2	270382	348641	19.20%	1.129%
44	14.782	2160	2164	2171	rVB3	148377	321038	17.68%	1.040%
45	14.882	2171	2181	2185	rBV3	288038	653604	35.99%	2.117%
46	14.964	2185	2195	2201	rBV4	670270	1644462	90.54%	5.326%
47	15.059	2201	2211	2216	rBV6	568135	1816305	100.00%	5.883%
48	15.217	2233	2238	2244	rVB	314209	569409	31.35%	1.844%
49	15.282	2244	2249	2251	rBV4	121114	201139	11.07%	0.651%
50	15.323	2252	2256	2261	rBV2	244821	428370	23.58%	1.387%
51	15.453	2270	2278	2286	rBV4	366677	1118491	61.58%	3.623%
52	15.606	2298	2304	2306	rBV5	220020	399258	21.98%	1.293%
53	15.706	2314	2321	2324	rBV	354730	719060	39.59%	2.329%
54	15.753	2325	2329	2333	rVV2	262190	446421	24.58%	1.446%
55	15.835	2340	2343	2354	rVB4	460826	1091114	60.07%	3.534%
56	15.953	2354	2363	2370	rBV3	374084	1020017	56.16%	3.304%
57	16.029	2372	2376	2380	rVV2	75217	134207	7.39%	0.435%
58	16.123	2386	2392	2395	rBV3	193262	413311	22.76%	1.339%
59	16.170	2395	2400	2407	rVB	744066	1496727	82.41%	4.848%
60	16.347	2425	2430	2436	rBV5	162241	336077	18.50%	1.088%
61	16.505	2447	2457	2465	rBV4	503337	1466918	80.76%	4.751%
62	16.717	2483	2493	2499	rBV4	698123	1692636	93.19%	5.482%

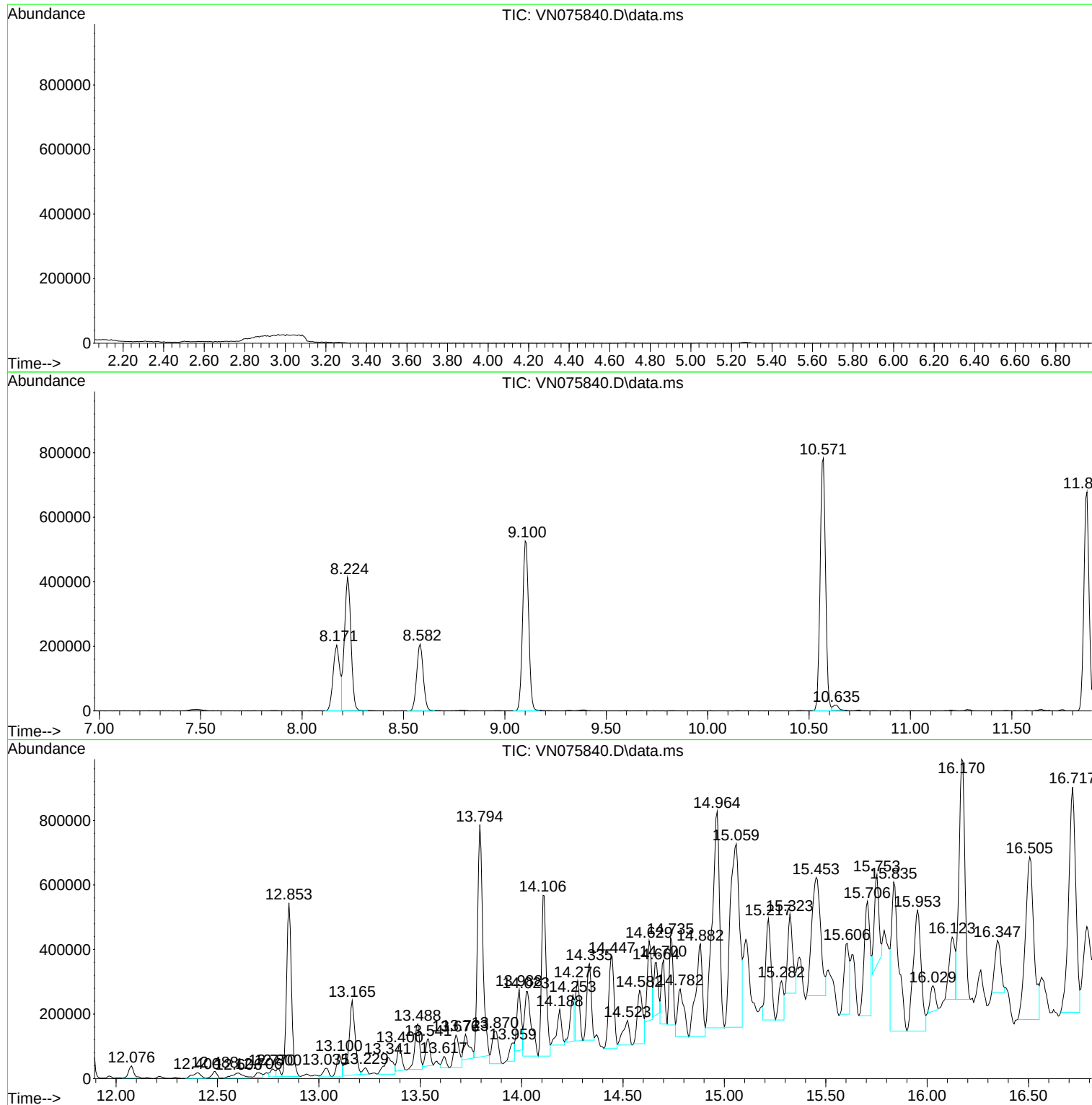
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_N
ClientSampleId :
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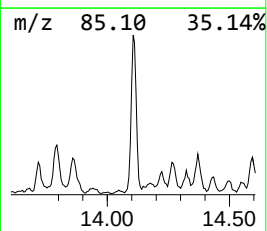
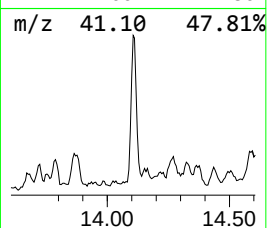
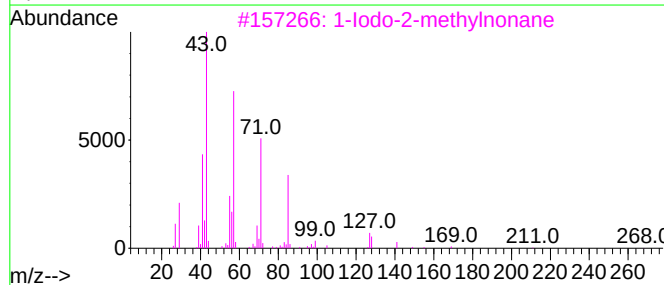
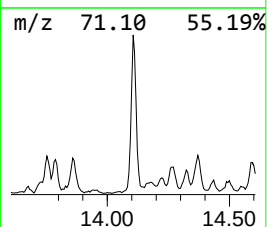
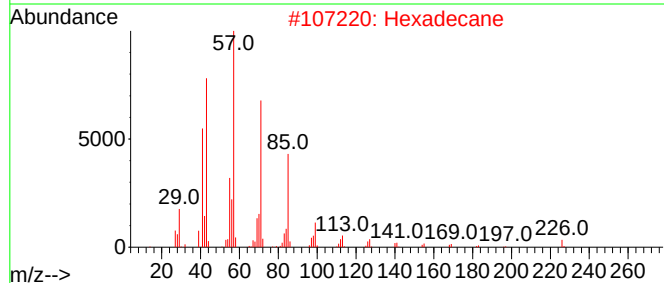
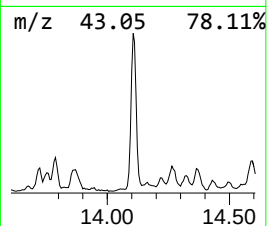
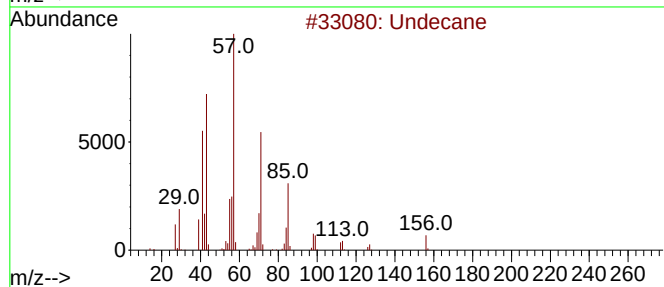
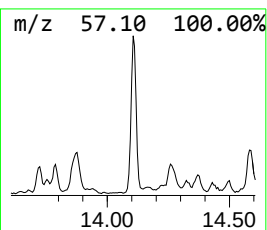
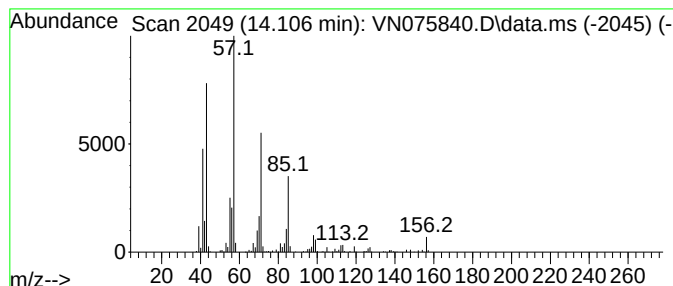
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	31.58 ug/l	815471	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Hexadecane			226	C16H34	000544-76-3	86
3	1-Iodo-2-methylnonane			268	C10H21I	1000101-47-9	72
4	Nonane			128	C9H20	000111-84-2	68
5	Tridecane			184	C13H28	000629-50-5	64



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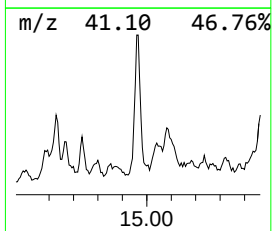
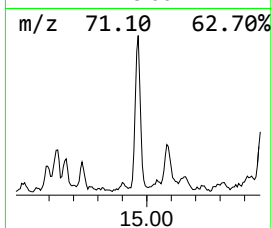
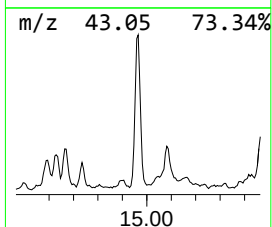
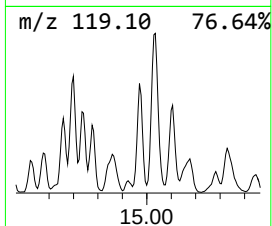
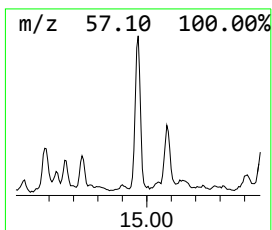
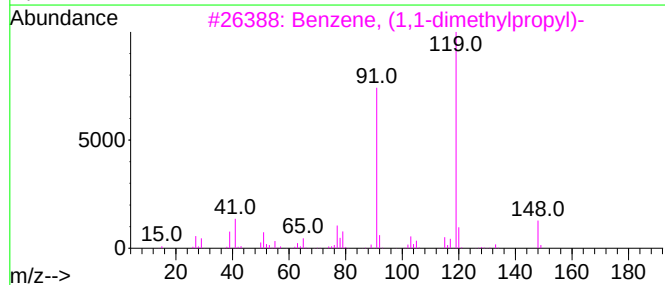
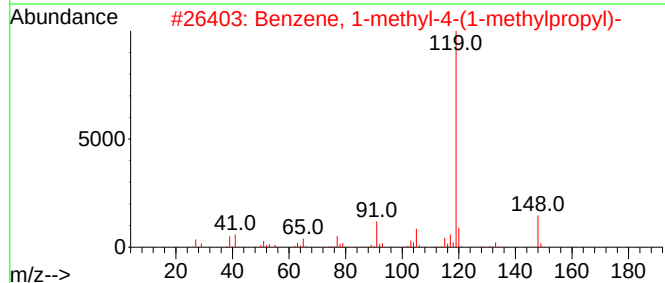
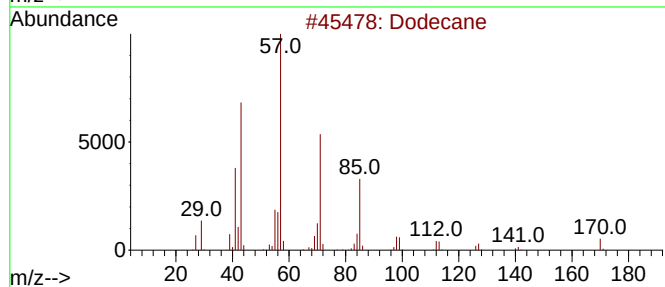
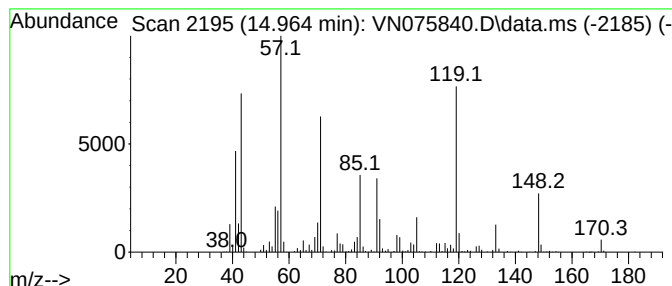
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	63.69 ug/l	1644460	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	89
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	46
3			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	41
4			Tetradecane	198	C14H30	000629-59-4	38
5			Hexadecane	226	C16H34	000544-76-3	30



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Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

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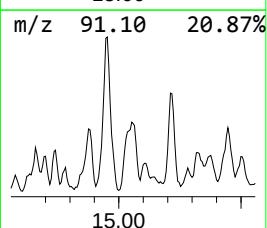
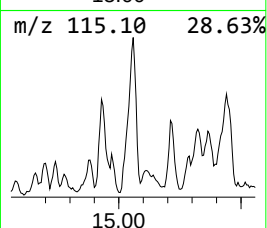
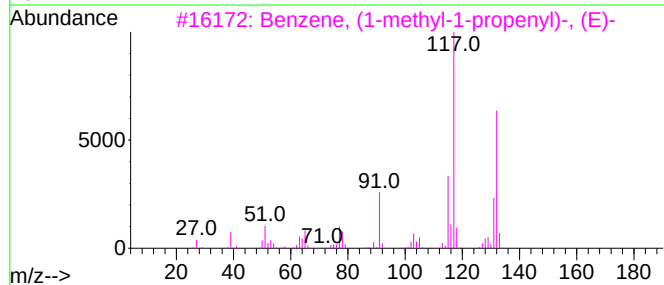
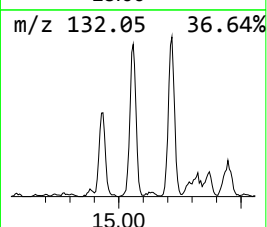
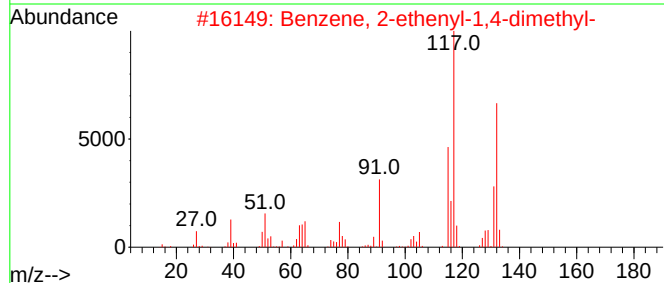
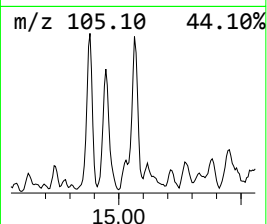
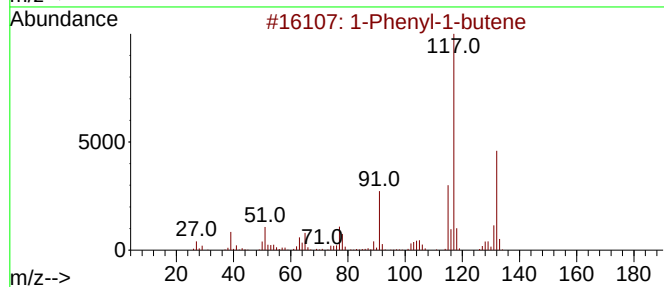
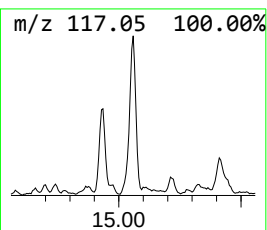
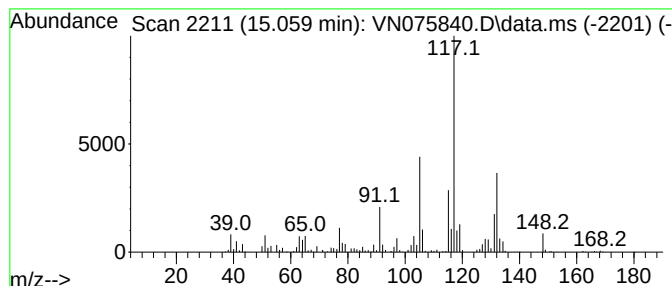
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenyl-1-butene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	70.34 ug/l	1816310	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	90



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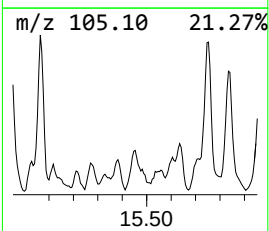
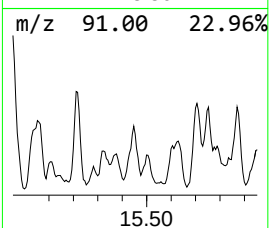
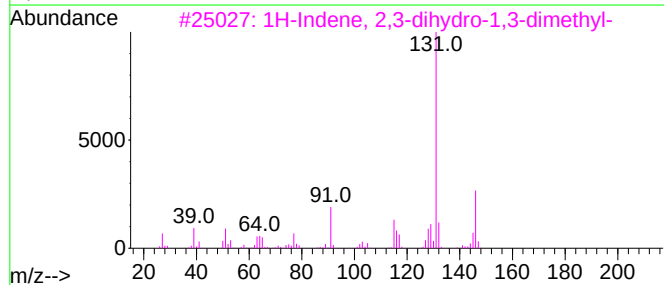
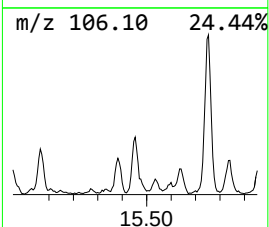
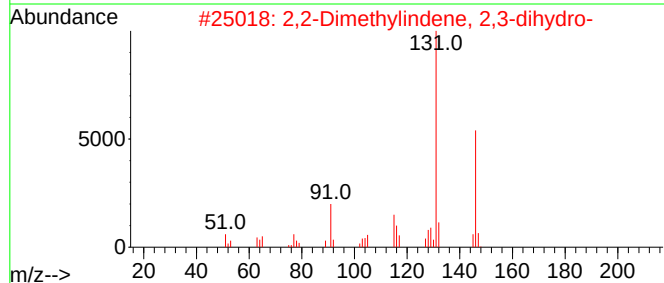
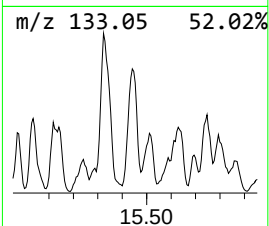
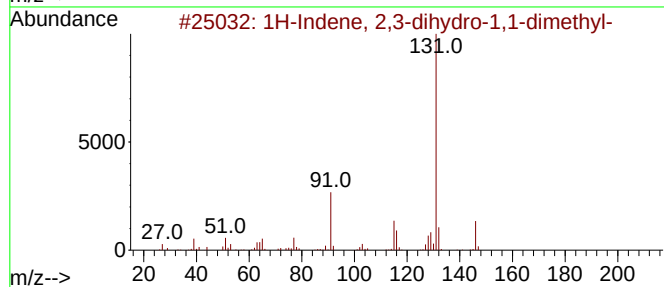
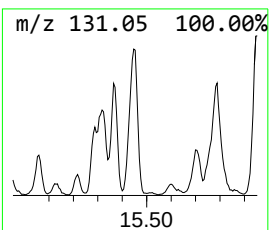
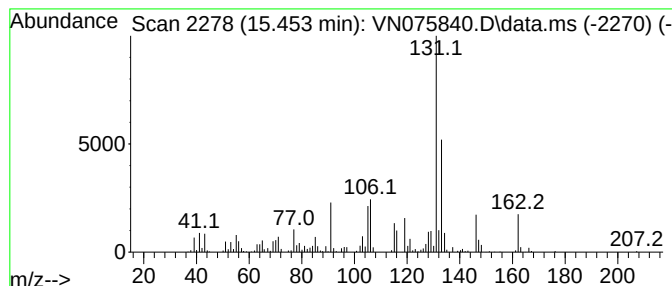
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1H-Indene, 2,3-dihydro-1,1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.453	43.32 ug/l	1118490	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	60
2			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	60
3			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	60
4			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	52
5			Cyclopropane, 1-chloro-1-methyl-...	166	C10H11Cl	1000161-07-9	49



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ClientSampleId :
31916

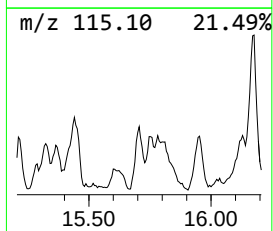
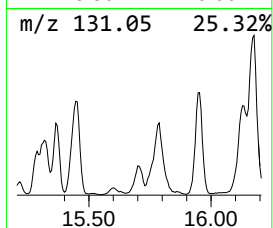
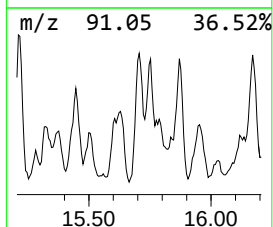
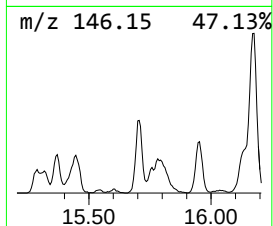
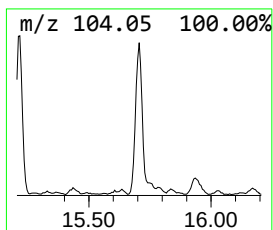
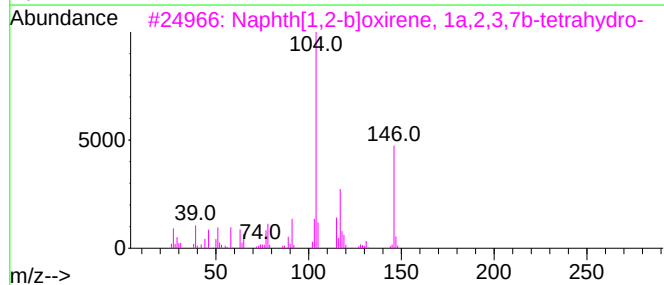
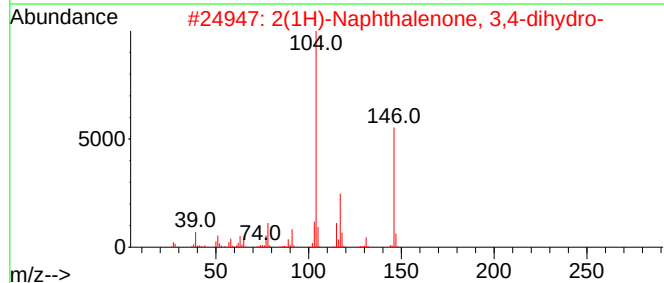
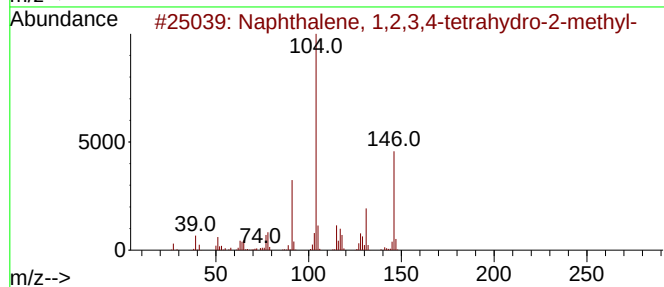
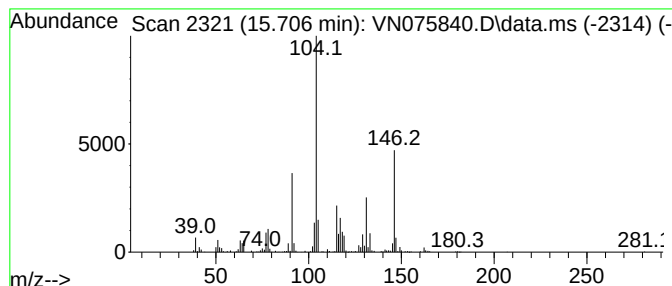
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.706	27.85 ug/l	719060	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	96
2			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	68
3			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	68
4			2,6-Piperidinedione, 3-phenyl-	189	C11H11NO2	014149-34-9	47
5			Benzene, 1-nonenyl-	202	C15H22	034426-61-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31916

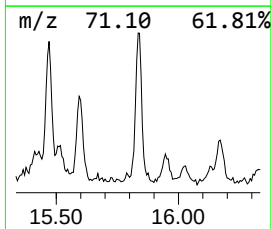
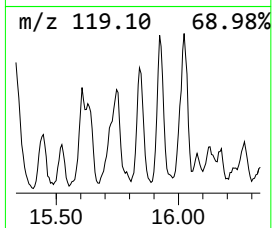
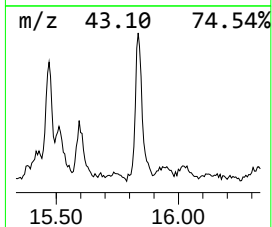
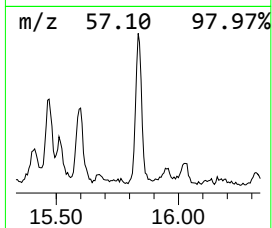
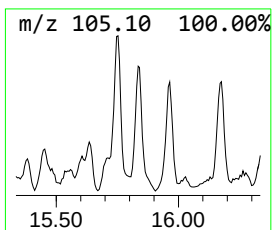
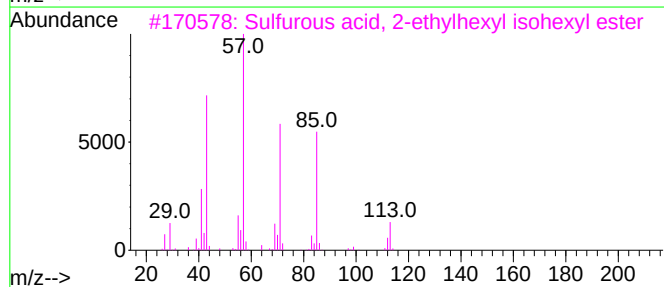
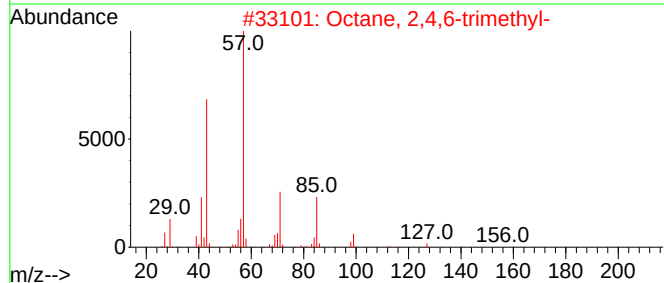
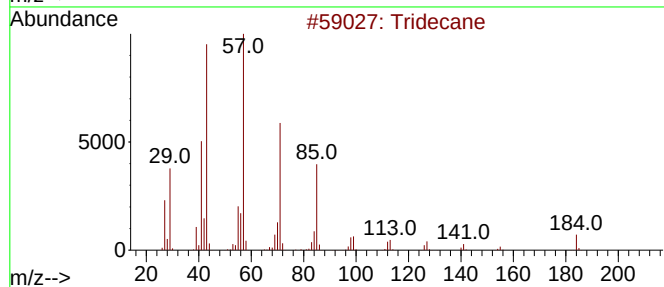
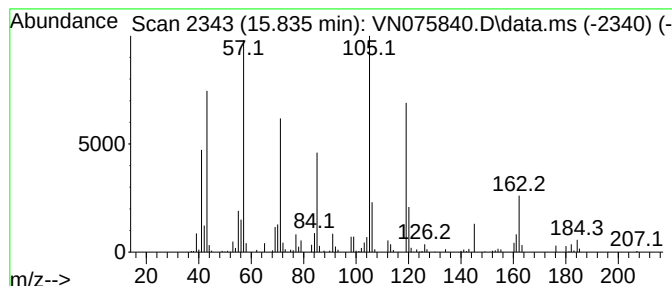
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	42.26 ug/l	1091110	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	74
2			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	30
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	30
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	27
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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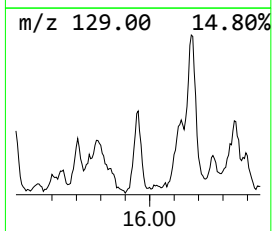
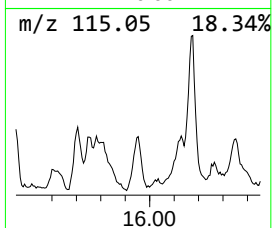
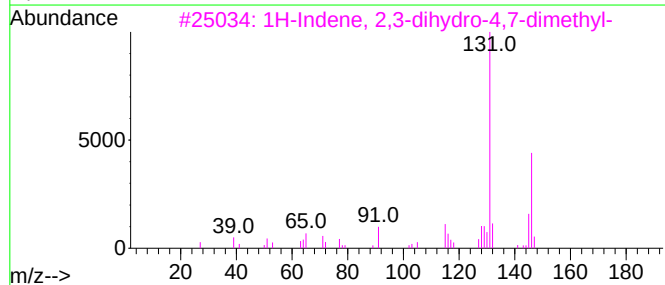
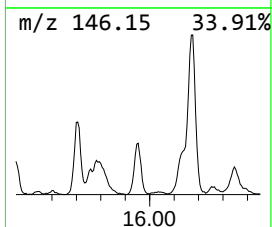
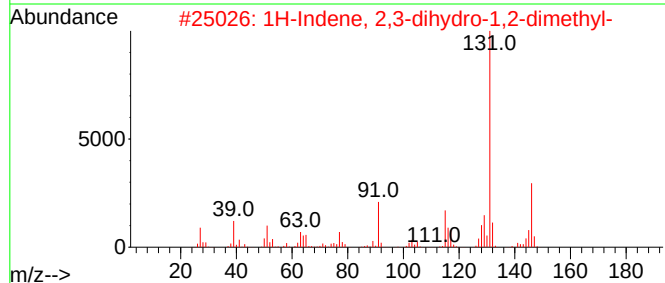
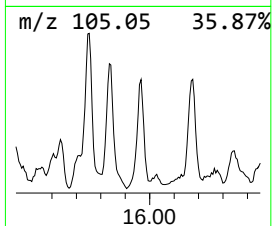
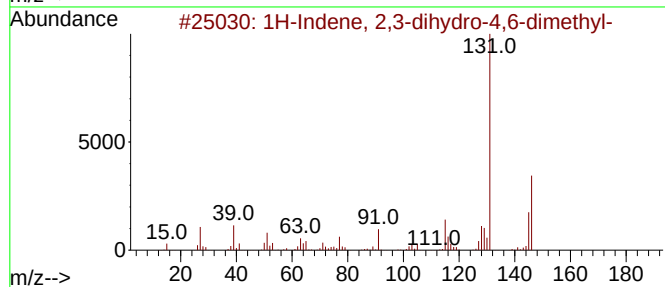
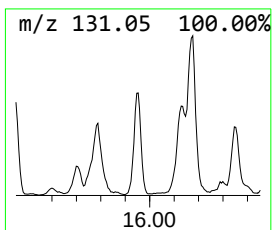
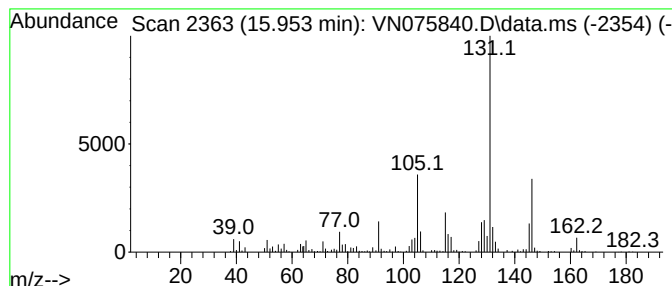
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1H-Indene, 2,3-dihydro-4,6-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.953	39.50 ug/l	1020020	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	93		
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	89		
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	89		
4	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	89		
5	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	86		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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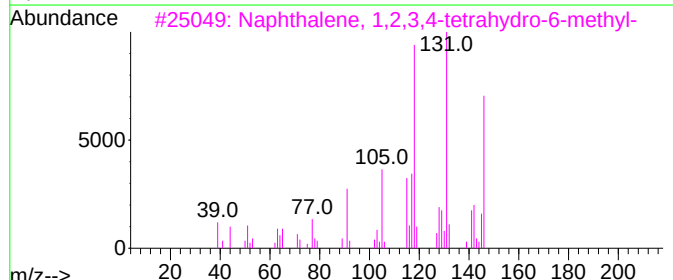
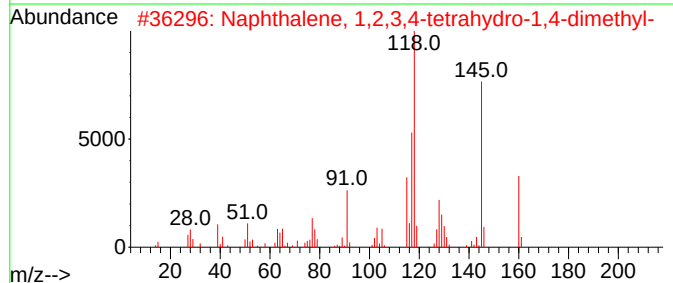
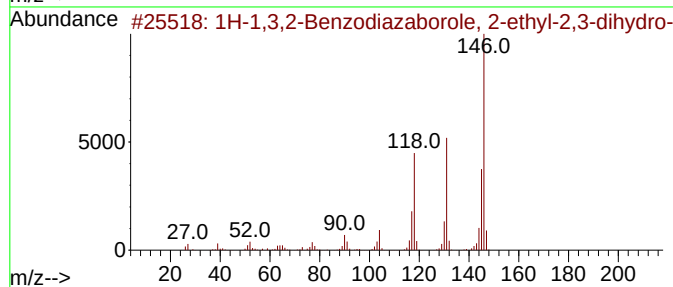
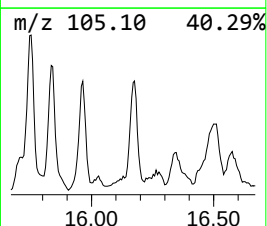
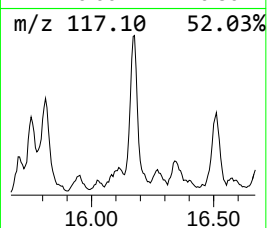
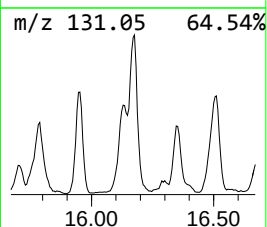
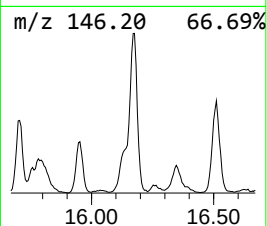
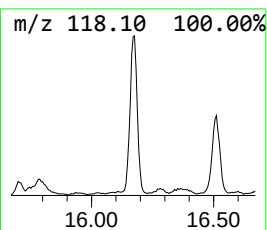
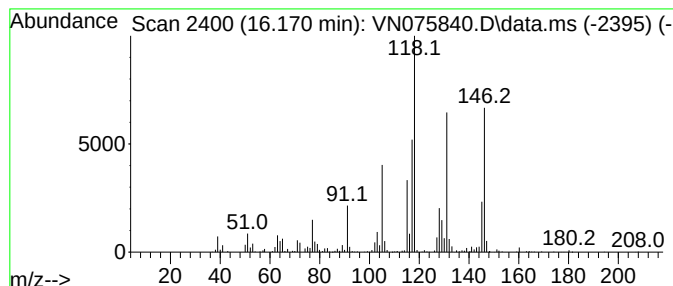
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1H-1,3,2-Benzodiazaborole, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	57.97 ug/l	1496730	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68		
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64		
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	58		
4	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	53		
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	52		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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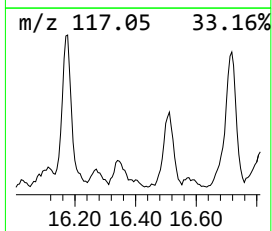
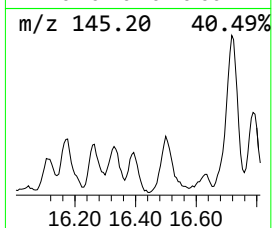
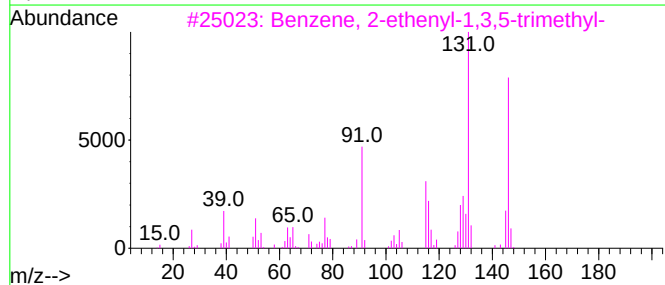
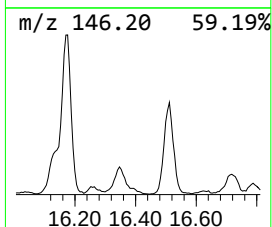
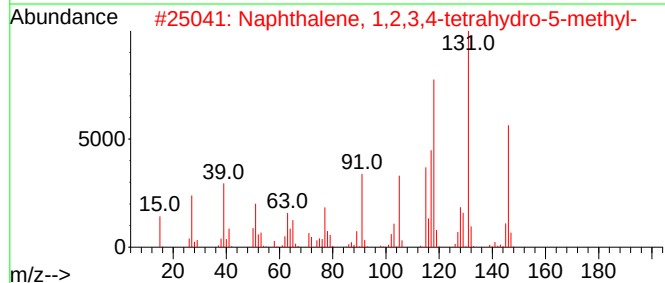
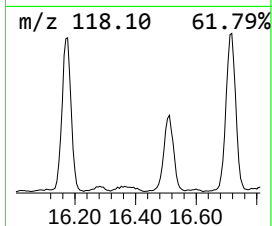
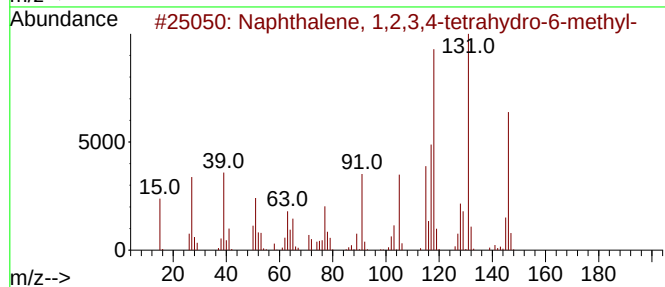
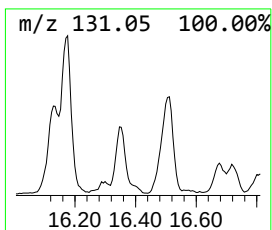
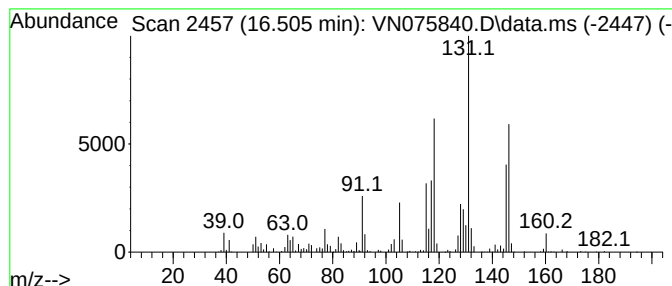
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	56.81 ug/l	1466920	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	90
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	83
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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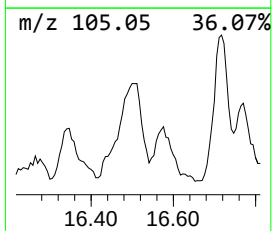
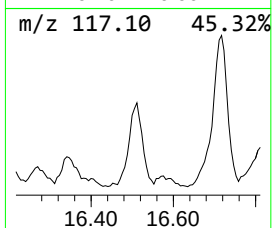
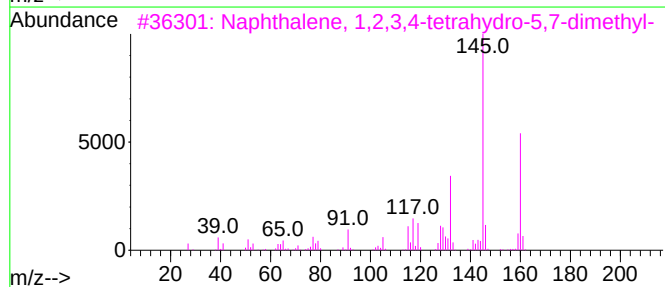
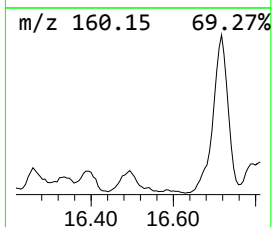
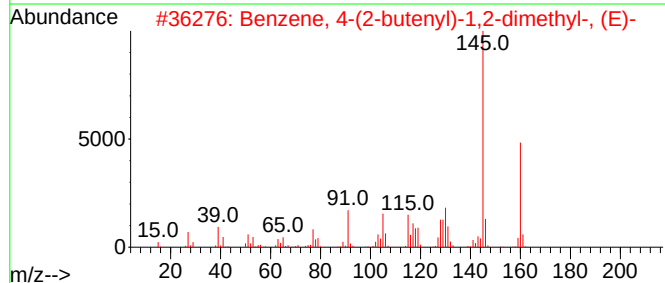
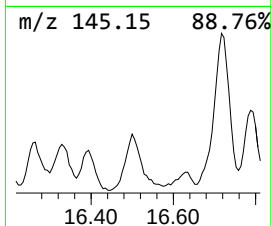
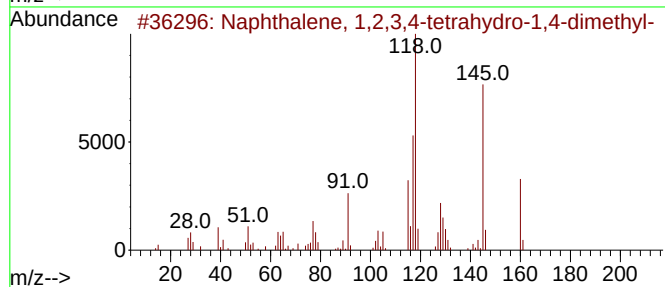
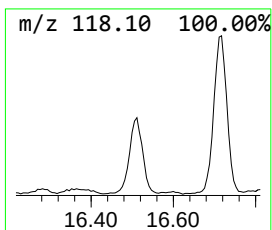
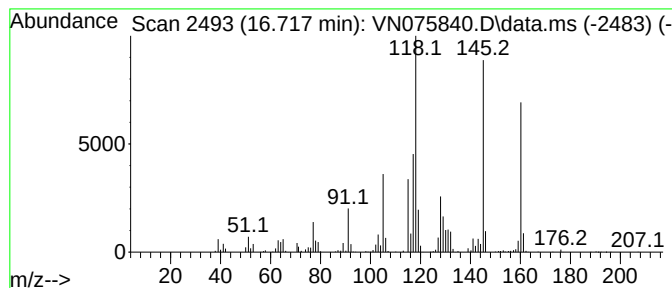
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.717	65.55 ug/l	1692640	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	78
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	78
4			Benzene, 1,2,4-trimethyl-5-(1-me...	160	C12H16	054340-84-0	70
5			4-Chloro-3-fluoroanisole	160	C7H6ClFO	000501-29-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075840.D
Acq On : 16 Dec 2022 12:13
Operator : JC\MD
Sample : N6036-01
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Dodecane	14.964	63.7	ug/l	1644460	4	13.794	1291030	50.0
1-Phenyl-1-butene	15.059	70.3	ug/l	1816310	4	13.794	1291030	50.0
1H-Indene, 2,3-...	15.453	43.3	ug/l	1118490	4	13.794	1291030	50.0
Naphthalene, 1,...	15.706	27.9	ug/l	719060	4	13.794	1291030	50.0
Tridecane	15.835	42.3	ug/l	1091110	4	13.794	1291030	50.0
1H-Indene, 2,3-...	15.953	39.5	ug/l	1020020	4	13.794	1291030	50.0
1H-1,3,2-Benzod...	16.170	58.0	ug/l	1496730	4	13.794	1291030	50.0
Naphthalene, 1,...	16.506	56.8	ug/l	1466920	4	13.794	1291030	50.0
Naphthalene, 1,...	16.717	65.5	ug/l	1692640	4	13.794	1291030	50.0